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Evaluation of the matrix element for positron impact ionization of atomic hydrogen near threshold in the effective charge model

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Abstract : We consider the evaluation of the matrix element for positron impact ionization of atomic hydrogen near threshold in the effective charge model wherein the final state is a product of two Coulomb functions—one for the attractive electron-proton and the other for the repulsive positron-proton interaction. Since the normalization factor of the part of the wave function corresponding to the repulsive interaction vanishes exponentially at threshold, it was thought uptill now that the matrix element would be almost insignificant over a considerable portion of the energy interval near the threshold We however show that the effect of this exponentially vanishing normalization factor is appropriately compensated for. To illustrate the striking contrast of our new finding with the earlier view we have calculated the total cross section for the 'no-screening' case where we get a square threshold law against the exponentially vanishing result of Geltman.

Keywords : Matrix element, positron impact ionization, effective charge model.

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Near the threshold, a very few studies have been done so far on the positron impact ionization. In the present work, we address the problem of the evaluation of the matrix element for positron impact ionization of hydrogen atom near threshold in the general effective charge model where the final state is represented by two appropriate Coulomb functions—one for the attractive and the other for the repulsive interaction, with two effective charges as seen by the emerging electron and the positron. The effective charges which take account of the correlation effect should be chosen in conformity with the Rudge-Seaton condition [1]. They are in general, functions of the energies and directions of the emitted particles.

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So long it has been thought that on account of the exponentially vanishing normalisation factor due to the repulsive positron-proton interaction, the matrix element would be almost insignificant over a considerable portion of the energy interval near the threshold. If so, then an effective charge model would be inapplicable to the calculation of positron impact ionization cross section near the threshold since it would lead to the very unphysical result just mentioned. In contrast, we have shown how the effect of the exponentially vanishing normalisation factor is appropriately compensated for, thus giving justification for the application of an adequate effective charge model to positron impact ionization near the threshold.

The total cross section in atomic unit for positron impact ionization of the hydrogen atom may be written as

$$\sigma = (1/k_0) \iint |M|^2 \, d\boldsymbol{k}_1 d\boldsymbol{k}_2 \, \delta(E - k_1^2/2 - k_2^2/2), \tag{1}$$

where
$$M = (1/2\pi) \left\langle \psi_f^- \left| 1/r_1 - 1/r_{12} \right| \psi_i \right\rangle. \tag{2}$$

The properly normalised final state wave function ψ_f^- here, near threshold, is given by

$$\psi_f^-(\boldsymbol{r}_1, \boldsymbol{r}_2) = \left[(\alpha_1 \alpha_2)^{1/2} \, e^{-\pi\alpha_1} / (2\pi)^{1/2} \right] \times e^{i\boldsymbol{k}_1 \cdot \boldsymbol{r}_1 + i\boldsymbol{k}_2 \cdot \boldsymbol{r}_2}$$
$$\times \, {}_1F_1 \left(i\alpha_1; 1; \; -i(k_1 r_1 + \boldsymbol{k}_1 \cdot \boldsymbol{r}_1) \right) \times {}_1F_1 \left(-i\alpha_2; 1; \; -i(k_2 r_2 + \boldsymbol{k}_2 \cdot \boldsymbol{r}_2) \right) \tag{3}$$

and the normalised initial state wave function is

$$\psi_i = (1/\pi^{1/2}) \, e^{-\lambda r_2 + i\boldsymbol{k}_0 \cdot \boldsymbol{r}_1}. \tag{4}$$

In (3) $\alpha_1 = z_1/k_1$ and $\alpha_2 = z_2/k_2$; $\boldsymbol{r}_1(\boldsymbol{r}_2)$ and $\boldsymbol{k}_1(\boldsymbol{k}_2)$ are respectively the position vector and momentum of the positron (electron), $\boldsymbol{k}_0$ is the incident momentum, z_1 and z_2 are the effective charges seen by the outgoing positron and the electron.

The matrix element M at threshold is given by

$$M = e^{-\pi\alpha_1} (\alpha_1 \alpha_2)^{1/2} \left(2\sqrt{2}\pi^2 \right)^{-1} \times I \tag{5}$$

with
$$I = \int e^{i\boldsymbol{k}_0 \cdot \boldsymbol{r}_1 - \lambda r_2} \, (1/r_1 - 1/r_{12}) \, e^{-i\boldsymbol{k}_1 \cdot \boldsymbol{r}_1 - i\boldsymbol{k}_2 \cdot \boldsymbol{r}_2}$$
$$\times \, {}_1F_1 \left(-i\alpha_1; 1; i(k_1 r_1 + \boldsymbol{k}_1 \cdot \boldsymbol{r}_1) \right) \times {}_1F_1 \left(i\alpha_2; 1; i(k_2 r_2 + \boldsymbol{k}_2 \cdot \boldsymbol{r}_2) \right) d\boldsymbol{r}_1 d\boldsymbol{r}_2. \tag{6}$$

Using the contour integral representation [2]

$${}_1F_1 (i\alpha; 1; z) = (1/2\pi i) \int e^{zt} \, p(\alpha, t) \, dt \tag{7}$$

where
$$p(\alpha, t) = t^{-1+i\alpha} (t-1)^{-i\alpha},$$

in (6), we get

$$I = (2\pi i)^{-2} \int \int dt_1\, dt_2\, \exp\left[i(\boldsymbol{k}_0 - \boldsymbol{k}_1).\, \boldsymbol{r}_1 - i\boldsymbol{k}_2.\, \boldsymbol{r}_2 - \lambda r_2\right] (1/r_1 - 1/r_{12})$$

$$\times \exp\left[it_1(k_1 r_1 + \boldsymbol{k}_1.\boldsymbol{r}_1) + it_2(k_2 r_2 + \boldsymbol{k}_2.\boldsymbol{r}_2)\right] p(-\alpha_1, t_1)\, p(\alpha_2, t_2)\, d\boldsymbol{r}_1 d\boldsymbol{r}_2$$

$$= \left[I_1 - I_2\right]. \tag{8}$$

We can evaluate analytically the integral I_1 which involves the interaction $1/r_1$ and show that its contribution is negligibly small. After performing the integrations with respect to $\boldsymbol{r}_1$ and $\boldsymbol{r}_2$ we have

$$I_1 = \underset{\eta \to 0+}{Lt} \frac{16\pi^2}{(2\pi i)^2} \frac{\delta}{\delta\lambda} \oint \left[dt_1 dt_2\, p(-\alpha_1, t_1)\, p(\alpha_2, t_2)\right] /$$

$$\left[\left[\left\{\boldsymbol{k}_0 - \boldsymbol{k}_1 (1 - t_1)\right\}^2 + (\eta - ik_1 t_1)^2\right] \times \left[\left|\boldsymbol{k}_2 (1 - t_2)\right|^2 + (\lambda - ik_2 t_2)^2\right]\right]. \tag{9}$$

On carrying out the contour integrations we get

$$I_1 = 16\pi^2 \left[(\boldsymbol{k}_0 - \boldsymbol{k}_1)^2\right]^{-1-i\alpha_1} \left[k_0^2 - k_1^2 - i0_+\right]^{i\alpha_1} \frac{\delta}{\delta\lambda}$$

$$\left[\left(k_2^2 + \lambda^2\right)^{-1+i\alpha_2} \times \left\{(\lambda - ik_2)\right\}^{-i\alpha_2}\right].$$

Putting $\lambda = 1$ after differentiation,

$$I_1 = 16\pi^2 \left[(\boldsymbol{k}_0 - \boldsymbol{k}_1)^2\right]^{-1-i\alpha_1} \left[k_0^2 - k_1^2 - i0_+\right]^{i\alpha_1} \times 2\left[(1 - z_2)\,(k_2 + i)^2\right]$$

$$\times \left[\left(k_2^2 + 1\right)\right]^{-2+i\alpha_2} \left[(1 - ik_2)\right]^{-1-i\alpha_2}.$$

Since $k_1 \to 0$, $k_2 \to 0$ and $|\boldsymbol{k}_0| = 1$ at threshold, we finally obtain

$$I_1 = 8\pi^2 (z_2 - 1)\, \exp\,(-2iz_1 \boldsymbol{k}_0.\boldsymbol{k}_1 - 2z_2). \tag{10}$$

The contribution of I_1 vanishes at threshold when it is multiplied by the normalisation factor $e^{-\pi\alpha_1}$.

Further, using the Fourier transformation technique, we can write I_2 which involves the interaction $1/r_{12}$ as

$$I_2 = \underset{\eta \to 0+}{Lt} \left[\frac{\delta^2}{\delta\lambda\, \delta\eta} \left[(1/2\pi i)^2 \oint dt_1 dt_2\, p(-\alpha_1, t_1)\, p(\alpha_2, t_2)\, J\right]\right], \tag{11}$$

where $$J = 8 \int d\boldsymbol{s} \left[\left\{\left|\boldsymbol{s} + \boldsymbol{k}_0 - \boldsymbol{k}_1 (1 - t_1)\right|^2 + (\eta - it_1 k_1)^2\right\}\right.$$

$$\left.\times \left\{\left|\boldsymbol{s} + (1 - t_2)\boldsymbol{k}_2\right|^2 + (\lambda - it_2 k_2)^2\right\}\right]^{-1} \tag{12}$$

We carry out the integrations in (11), differentiate the result with respect to λ and η, and obtain

$$I = -32\, z_1 \int ds\left[(1+z_2)s^2 + 2iz_2(s.\hat{k}_2) + 2z_2 s.k_2 - (1-z_2)(k_2+i)^2\right]$$
$$\times \left[(s+k_0-k_1)^2\right]^{-1-i\alpha_1} \left[(s+k_0)^2 - k_1^2 - 2i\eta k_1\right]^{-1+i\alpha_1}$$
$$\times \left[(s+k_2)^2+\lambda^2\right]^{-2+i\alpha_2} \cdot \left[s^2+(\lambda-ik_2)^2\right]^{-1-i\alpha_2} \times s^{-2} \qquad (13)$$

In the expression $\left[(s+k_0)^2 - k_1^2 - 2i\eta k_1\right]^{-1+i\alpha_1}$ of (13), if we put $s + k_0 - k_1 = P$ and consider the limit $\eta \to 0_+$, we get

$$\underset{\eta\to 0+}{Lt} \left[(s+k_0)^2 - k_1^2 - 2i\eta k_1\right] = P(P-X-i0_+), \text{ where } X = -2k_1.\hat{P}.$$

On account of the negative imaginary infinitesimal phase $-i0_+$, in the very small region where $P < X$, we have

$$\left[(s+k_0)^2 - k_1^2 - 2i\eta k_1\right]^{-n+i\alpha_1} = (-1)^n e^{\pi\alpha_1} P^{-n+i\alpha_1} (X-P)^{-n+i\alpha_1}. \qquad (14)$$

Thus, the contribution of this region only is significant at threshold since the effect of the vanishingly small normalisation factor $e^{-\pi\alpha_1}$ in (5) is compensated by the factor $e^{\pi\alpha_1}$ present there.

In this small region, we can consider $s^2 \approx k_0^2$, $s.\hat{k}_2 \approx -k_0.\hat{k}_2$

Further in (13) when $k_2 \to 0$, we can write

$$(s^2+\lambda^2+2\,s.k_2)^{-2+i\alpha_2}\,(s^2+\lambda^2-2\,i\lambda k_2)^{-1-i\alpha_2}$$
$$\approx \left(k_0^2+\lambda^2\right)^{-3} e^{\left[-2i\hat{k}_0\,\hat{k}_2 z_2/(k_0^2+\lambda^2)\right]} \times e^{\left[-2\lambda z_2/(k_0^2+\lambda^2)\right]} \qquad (15)$$

(since $\alpha_2 = z_2/k_2$).

Considering only the dominant contribution, we get after integration over the azimuthal angle and putting $\lambda = 1$, $k_0 = 1$.

$$I = (8\pi/k_1)(1-iC)\exp\left[-z_2 - iC + \pi\alpha_1\right]$$
$$\times \int_{\varepsilon}^{2k_1} dP[P]^{-1-i\alpha_1} \int_{P+\delta}^{2k_1} (X-P)^{-1+i\alpha_1}\, dX, \qquad (16)$$

where $C = z_2\hat{k}_0.\hat{k}_2$, and ε, δ are infinitestmal positive quantities.

Integrating over X, we have

$$I = (8\pi/iz_1)(1-iC)\exp\left[-z_2 - iC + \pi\alpha_1\right] \int dP\,[P]^{-1-i\alpha_1}$$
$$\left[(2k_1-P)^{i\alpha_1} - \delta^{i\alpha_1}\right]. \qquad (17)$$

Now $$\underset{\varepsilon \to 0+}{Lt} \int_{\varepsilon}^{2k_1} dP P^{-1-i\alpha_1} (2k_1 - P)^{i\alpha_1} = B(-i\alpha_1, 1 + i\alpha_1)$$

and this as we know is proportional to exp $(-\pi\alpha_1)$.

So finally we have

$$I = -(8\pi k_1(1 - iC)/z_1^2) \exp\left[-z_2 - iC + \pi\alpha_1\right] \times \left[(\delta/2k_1)^{i\alpha_1} - (\delta/\varepsilon)^{i\alpha_1}\right] \tag{18}$$

and hence,

$$|M|^2 = (2^4/\pi^2)(k_1/k_2)(z_2/z_1^3) \exp(-2z_2)(1 + z_2^2 \cos^2\theta_2). \tag{19}$$

With the help of (19) we can easily calculate the triple differential cross sections.

To obtain the total cross section however, one should know explicitly the dependence of the effective charges z_1 and z_2 on the momenta $\boldsymbol{k}_1$ and $\boldsymbol{k}_2$ of the particular model to be used.

Just to illustrate the striking contrast of our new finding with the earlier view, we calculate here the total cross section for the Geltman model [3] of no screening ($z_1 = z_2 = 1$) which is a simple model amenable to an easy calculation though it is not quite accurate as it does not satisfy the Rudge-Seaton condition. Substituting in (1) the expression for $|M|^2$ of (19) with $z_1 = z_2 = 1$ and carrying out the integrations over $\boldsymbol{k}_1$ and $\boldsymbol{k}_2$ we finally obtain the threshold ionization cross section as

$$\sigma = (2^{10}/3) \exp(-2)E^2. \tag{20}$$

This square threshold law is quite different from Geltman's exponentially vanishing result. It should be noted that the Geltman model for the corresponding case of electron impact ionization yields a linear threshold law for the total cross section.

For electron impact ionization near the threshold, the Wannier model [4] based on the classical theory, gives a threshold law $\sigma \sim E^{1.127}$ for hydrogen atom which is in general, considered to be more or less satisfactory. Quantum mechanical extension of this model was attempted by Peterkop [5], Rau [6] and others. Klar [7] has extended the Wannier model to positron impact ionization and obtained analytically a threshold law $\sigma \sim E^{2.65}$ for hydrogen atom. Modification of the Wannier threshold law for small but finite energy excess above the threshold has been considered by Kazansky *et al* [8]. For positron impact, the Wannier threshold law is rather controversial. Dimitrijevic and Grujic [9] have obtained a threshold law $\sigma \sim E^{1.64}$ for positron impact ionization of hydrogen atom by their classical trajectory study. The classical trajectory Monte Carlo calculations of Wetmore and Olson [10] on the other hand, agree with the power law $\sigma \sim E^{3.01}$. Temkin [11] by his quantum mechanical approach has arrived at modulated linear threshold laws both for electron and positron impact.

At the excess energy 1.4 eV (lowest energy known to us) the experimental value [12] (from graph) is $\sigma \approx 1.8 \times 10^{-17}$ cm^2 nearly five times the value 0.35×10^{-17} cm^2 calculated from (20). In view of the fact that the simple Geltman model is not accurate enough, we do not expect a quantitative agreement of the calculated numerical value with experimental result. However, we note that both are of the same order of magnitude. No other theoretical value is available at such a low energy, to our knowledge. It should be noted that the Wannier law does not give the absolute magnitude of the cross section which is required for a quantitative comparison with experiment.

Precise measurement of the ionization cross section very close to the threshold, is urgently required for a comparison with the theoretical prediction of an adequate effective charge model.

References

[1] M R H Rudge and M J Seaton *Proc. Roy. Soc* **A83** 262 (1965)

[2] A Nordsieck *Phys Rev* **93** 785 (1954)

[3] S Geltman *J. Phys* **B16** 1525 (1983)

[4] G Wannier *Phys. Rev.* **90** 817 (1954)

[5] R Peterkop *J. Phys* **B4** 513 (1971)

[6] A R P Rau *Phys. Rev* **A4** 207 (1971)

[7] H Klar *J Phys.* **B14** 4165 (1981)

[8] A K Kazansky, V N Ostrovsky and L Yu Sergeeva *Z. Phys* **D33** 181 (1995)

[9] M S Dimitrijevic and P V Grujic *J Phys.* **B16** 297 (1983)

[10] A W Wetmore and R E Olson *Phys Rev.* **A34** 2822 (1986)

[11] A Temkin *Phys. Rev Lett* **49** 366 (1982)

[12] G O Jones, M Charlton, J Slevin, G Laricchia, A Kover, M R Poulsen and S N Chormaic *J. Phys.* **B26** L483 (1993)